Chapter 59 - **SANS RESOLUTION WITH SLIT GEOMETRY**

Slit geometry is sometime used in order to obtain high resolution in one direction. This enhances the flux-on-sample but introduces drastic smearing effects in the other direction. The two instruments that use slit geometry are the VSANS instrument ("V" is for "very) and the Bonse-Hart USANS instrument ("U" is for "ultra"). The resolution function for slit geometry is discussed here.

1. VARIANCE OF THE Q RESOLUTION

Recall the following result that was derived for circular aperture geometry (Mildner-Carpenter, 1984):

$$\left[\sigma_Q{}^2\right]_{geo} = \frac{4\pi^2}{\lambda^2}\frac{\sigma_x{}^2 + \sigma_y{}^2}{L_2{}^2} \qquad (1)$$

with:

$$\sigma_x{}^2 = \left(\frac{L_2}{L_1}\right)^2 < x^2 >_1 + \left(\frac{L_1 + L_2}{L_1}\right)^2 < x^2 >_2 + < x^2 >_3$$

$$\sigma_y{}^2 = \left(\frac{L_2}{L_1}\right)^2 < y^2 >_1 + \left(\frac{L_1 + L_2}{L_1}\right)^2 < y^2 >_2 + < y^2 >_3$$

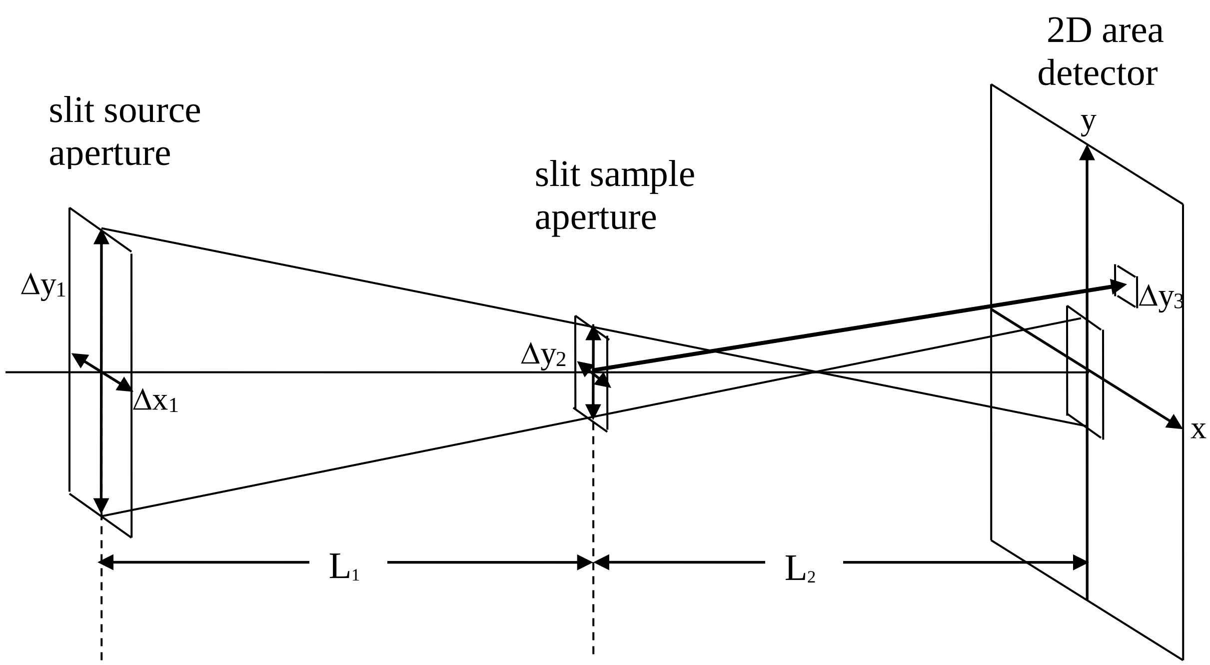

Figure 1: SANS slit geometry with rectangular source and sample apertures and 2D area detector cells. This figure is not to scale. Cartesian coordinates are used to characterize the three vertical (source, sample and detector) planes.

In the case of slit geometry, the various averages are calculated as follows. The horizontal slit openings for the source and sample apertures are defined as Δx_1 and Δx_2 and the vertical slit openings are defined as Δy_1 and Δy_2. Δx_3 and Δy_3 represent the detector cell dimensions. The various averages can be readily calculated.

$$< x^2 >_1 = \frac{\int_{-\Delta x_1/2}^{\Delta x_1/2} dx\, x^2}{\int_{-\Delta x_1/2}^{\Delta x_1/2} dx} = \frac{1}{3}\left(\frac{\Delta x_1}{2}\right)^2 = \frac{\Delta x_1{}^2}{12} \qquad (2)$$

$$< x^2 >_2 = \frac{\Delta x_2{}^2}{12};\ < x^2 >_3 = \frac{\Delta x_3{}^2}{12}$$

$$< y^2 >_1 = \frac{\Delta y_1{}^2}{12};\ < y^2 >_2 = \frac{\Delta y_2{}^2}{12};\ < y^2 >_3 = \frac{\Delta y_3{}^2}{12}.$$

The collimation contribution for slit geometry is similar to that for circular apertures with slightly different terms. Note that the gravity term appears only in the vertical y direction.

$$\sigma_Q{}^2 = \sigma_{Qx}{}^2 + \sigma_{Qy}{}^2 \qquad (3)$$

$$\sigma_{Qx}{}^2 = \left(\frac{2\pi}{\lambda L_2}\right)^2\left[\left(\frac{L_2}{L_1}\right)^2\frac{\Delta x_1{}^2}{12} + \left(\frac{L_1+L_2}{L_1}\right)^2\frac{\Delta x_2{}^2}{12} + \frac{\Delta x_3{}^2}{12}\right] + Q_x{}^2\,\frac{1}{6}\left(\frac{\Delta\lambda}{\lambda}\right)^2$$

$$\sigma_{Qy}{}^2 = \left(\frac{2\pi}{\lambda L_2}\right)^2\left[\left(\frac{L_2}{L_1}\right)^2\frac{\Delta y_1{}^2}{12} + \left(\frac{L_1+L_2}{L_1}\right)^2\frac{\Delta y_2{}^2}{12} + \frac{\Delta y_3{}^2}{12}\right] + Q_y{}^2\,\frac{1}{6}\left(\frac{\Delta\lambda}{\lambda}\right)^2 + \frac{4\pi^2}{\lambda^2 L_2{}^2} A^2\lambda^4\,\frac{2}{3}\left(\frac{\Delta\lambda}{\lambda}\right)^2$$

$$A = L_2(L_1 + L_2)\frac{gm^2}{2h^2}.$$

Here L_1 and L_2 are the source-to-sample and sample-to-detector distances.

Note that only the $<x^2>$ terms are different from the pinhole geometry case.

2. MINIMUM Q WITH SLIT GEOMETRY

The minimum Q achieved with slit geometry has horizontal and vertical components. The horizontal component is the lowest because collimation is often tightened in that direction. Slits are aligned in the vertical direction to avoid gravity effects. The Q_{min} values are similar to the case of pinhole geometry and are summarized here.

$$Q_{min}^{X} = \frac{2\pi}{\lambda}\frac{X_{min}}{L_2} \text{ and } Q_{min}^{Y} = \frac{2\pi}{\lambda}\frac{Y_{min}}{L_2} \tag{4}$$

$$X_{min} = \frac{L_2}{L_1}\frac{\Delta x_1}{2} + \frac{L_1+L_2}{L_1}\frac{\Delta x_2}{2} + \frac{\Delta x_3}{2}$$

$$Y_{min} = Y_{min}^{0} + 2A\lambda^2\left(\frac{\Delta\lambda}{\lambda}\right)$$

$$Y_{min}^{0} = \frac{L_2}{L_1}\frac{\Delta y_1}{2} + \frac{L_1+L_2}{L_1}\frac{\Delta y_2}{2} + \frac{\Delta y_3}{2}.$$

Gravity affects the vertical direction which is of no value because it is highly smeared due to the open collimation in that direction.

3. APPLICATION TO A SPECIFIC CASE

Consider the following instrument configuration with slit geometry:

$$\begin{aligned}
\Delta x_1 &= 0.25 \text{ cm} \\
\Delta y_1 &= 2.5 \text{ cm} \\
\Delta x_2 &= 0.05 \text{ cm} \\
\Delta y_2 &= 0.5 \text{ cm} \\
\Delta x_3 &= 0.05 \text{ cm} \\
\Delta y_3 &= 0.5 \text{ cm} \\
L_1 &= 15 \text{ m} \\
L_2 &= 15 \text{ m} \\
\lambda &= 12 \text{ Å} \\
\frac{\Delta\lambda}{\lambda} &= 15 \%.
\end{aligned} \tag{5}$$

Therefore:

$$\begin{aligned}
A &= 0.0138 \text{ cm/Å}^2 \\
\sigma_x^2 &= 0.00625 \text{ cm}^2 \\
\sigma_y^2 &= 0.625 \text{ cm}^2.
\end{aligned} \tag{6}$$

So that:

$$\sigma_{Qx}^{\ 2} = 7.61*10^{-10} + 0.0037\,Q_x^{\ 2} \text{ (in units of Å}^{-2}\text{)} \tag{7}$$
$$\sigma_{Qy}^{\ 2} = 8.34*10^{-8} + 0.0037\,Q_y^{\ 2} \text{ (in units of Å}^{-2}\text{).}$$

Moreover,

$$Q_{min}^{\ X} = 0.00014\,\text{Å}^{-1} \tag{8}$$
$$Q_{min}^{\ Y} = 0.0016\,\text{Å}^{-1}.$$

In this case, the horizontal resolution is very good but the vertical one is poor.

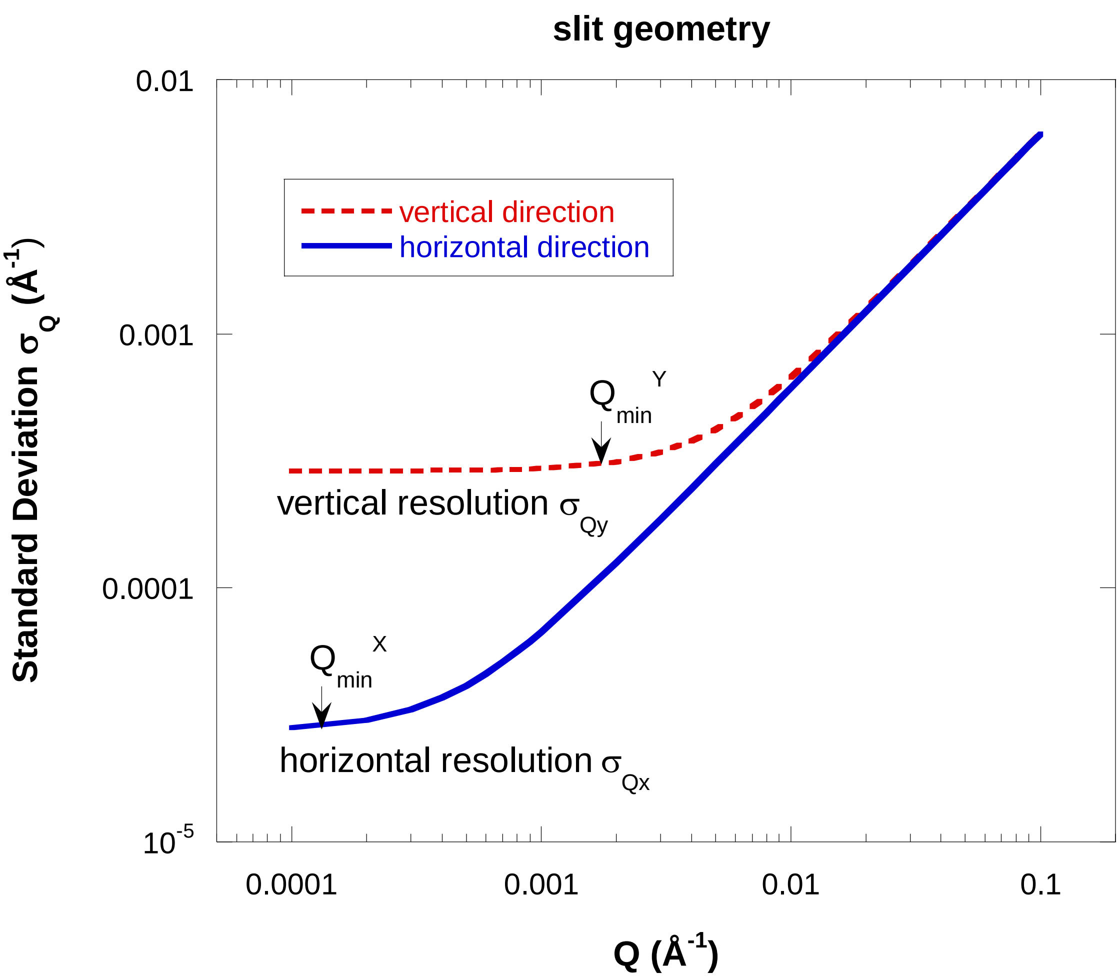

Figure 2: Standard deviation of the instrumental resolution for slit geometry. Resolution is tight in the horizontal direction and "opened up" in the vertical direction to enhance flux on sample. The values of Q_{min} are also indicated.

4. SLIT SMEARING CORRECTION

When correcting data with slit smearing, the horizontal and vertical directions are decoupled as follows:

$$R(Q,Q') = R(Q-Q') = R(Q_x-Q'_x)\, R(Q_y-Q'_y) \tag{9}$$

$$R(Q_x - Q_x') = \sqrt{\frac{1}{2\pi\sigma_{Qx}^2}}\, \exp\left[-\frac{(Q_x - Q'_x)^2}{2\sigma_{Qx}^2}\right]$$

$$R(Q_y - Q_y') = \sqrt{\frac{1}{2\pi\sigma_{Qy}^2}}\, \exp\left[-\frac{(Q_y - Q'_y)^2}{2\sigma_{Qy}^2}\right].$$

The resolution integral becomes:

$$\left[\frac{d\Sigma(Q)}{d\Omega}\right]_{\text{smeared}} = \int_{-\infty}^{\infty} dQ'_x \int_{-\infty}^{\infty} dQ'_y R(Q_x - Q_x') R(Q_y - Q_y') \left[\frac{d\Sigma(Q'_x, Q'_y)}{d\Omega}\right]_{\text{un-smeared}} \tag{10}$$

Slits are usually very small in the horizontal direction so that $R(Q_x-Q'_x) = \delta(Q_x-Q'_x)$ where δ is the Dirac Delta function. In the vertical direction the resolution is sometime replaced by a uniform "box" function (Barker et al, 2005):

$$R(Q_y-Q'_y) = 0 \text{ for } |Q_y-Q'_y| < \frac{-\Delta Q_y}{2} \text{ or } |Q_y-Q'_y| > \frac{\Delta Q_y}{2} \tag{11}$$

$$R(Q_y-Q'_y) = \frac{1}{\Delta V} \text{ for } \frac{-\Delta Q_y}{2} \le |Q_y-Q'_y| \le \frac{\Delta Q_y}{2}.$$

Within this "infinitely thin slit" approximation, the resolution integral becomes simpler.

$$\left[\frac{d\Sigma(Q)}{d\Omega}\right]_{\text{smeared}} = \frac{1}{\Delta Q_y} \int_0^{\Delta Q_y} dQ'_y \left[\frac{d\Sigma(Q_x, Q'_y)}{d\Omega}\right]_{\text{un-smeared}} \tag{12}$$

$$= \frac{1}{\Delta Q_y} \int_0^{\Delta Q_y} dQ'_y \left[\frac{d\Sigma(\sqrt{Q_x^2 + Q'^2_y})}{d\Omega}\right]_{\text{un-smeared}}.$$

We have made use of the following property of the Dirac Delta function:

$$\int_{-\infty}^{\infty} dQ'_x \delta(Q_x - Q'_x) \left[\frac{d\Sigma(Q'_x, Q'_y)}{d\Omega}\right]_{\text{un-smeared}} = \left[\frac{d\Sigma(Q_x, Q'_y)}{d\Omega}\right]_{\text{un-smeared}}. \tag{13}$$

The desmearing procedure becomes a simple 1D integration.

REFERENCES

D.F.R. Mildner, and J.M. Carpenter, ”Optimization of the Experimental Resolution for SAS”, J. Appl. Cryst. 17, 249-256 (1984)

J.G. Barker, C.J. Glinka, J.J. Moyer, M.H. Kim, A.R. Drews, and M. Agamalian,” Design and Performance of a Thermal-Neutron Double-Crystal Diffractometer for USANS at NIST”, J. Appl. Cryst. 38: 1004-1011 (2005).

QUESTIONS

1. What is the main difference in the variance of the resolution function between the cases with circular apertures and with slit geometry?
2. What are the main advantage and disadvantage of slit geometry?

ANSWERS

1. The main difference in the variance of the resolution function σ_Q between the cases with circular apertures and with slit geometry is in the averaging process involved in the calculation of the geometry contribution; for a circular aperture of radius R_1, the average is $< x^2 >_1 = \frac{R_1^2}{4}$, whereas for a slit of width Δx_1, it is $< x^2 >_1 = \frac{1}{3}\left(\frac{\Delta x_1}{2}\right)^2$.
2. The advantage of slit geometry is increased flux-on-sample in the relaxed collimation direction. The disadvantage of the slit geometry is the drastic smearing effect.